

1-Methyl-6-(2-methylphenyl)-1,6-dihydro-3-pyridinecarbonitrile  
27531-42-6 | DTXSID60299776

Model Performance

Model

Data

Weighted KNN model

| 5-fold CV (75%) |      | Training (75%) |      | Test (25%) |      |
|-----------------|------|----------------|------|------------|------|
| Q2              | RMSE | R2             | RMSE | R2         | RMSE |
| 0.89            | 0.25 | 0.88           | 0.26 | 0.75       | 0.38 |

## Model Results

**Predicted value:** 3.53 days

**Global applicability domain:** Outside

**Local applicability domain index:** 3.19e-01

**Confidence level:** 9.31e-01

## Nearest Neighbors from the Training Set

Image not found

1-Methyl-2-propylbenzene

**Measured:** 12.5

**Predicted:** 3.17

Image not found

3-Ethyltoluene

**Measured:** 12.5

**Predicted:** 3.26

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1,3-Dimethyl-4-ethylbenzene

**Measured:** 24.3

**Predicted:** 3.89

Image not found

1-Ethyl-2-methylbenzene

**Measured:** 24.3

**Predicted:** 3.88

Image not found

Propylbenzene

**Measured:** 24.3

**Predicted:** 4.02